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chain nodes :

7 8 9 10 11 12 13 14 15 16 17 24 25 26 27 28 29 30 31 32 33 40 41 48 49 52 53 54 55 56 57 58 59 60 61 62 63 64 ring nodes : 1 2 3 4 5 6 18 19 20 21 22 23 34 35 36 37 38 39 42 43 44 46 47 chain bonds : 19 - 3135-55 36 - 5236-53 37-58 37-59 38-40 39-56 39-57 42-62 42-63 43-49 44-64 44 - 6545 - 4847-60 47-61 ring bonds : $1 - 2 \quad 1 - 6 \quad 2 - 3 \quad 3 - 4 \quad 4 - 5 \quad 5 - 6 \quad 18 - 19 \quad 18 - 23 \quad 19 - 20 \quad 20 - 21 \quad 21 - 22 \quad 22 - 23 \quad 34 - 35$ $34 - 39 \quad 35 - 36 \quad 36 - 37 \quad 37 - 38 \quad 38 - 39 \quad 42 - 43 \quad 42 - 47 \quad 43 - 44 \quad 44 - 45 \quad 45 - 46 \quad 46 - 47 \quad 43 - 44 \quad 44 - 45 \quad 45 - 46 \quad 46 - 47 \quad 48 - 48 \quad 48$ exact/norm bonds : 10/573,723 08/25/2009 STN: SEARCH

exact bonds : $1 - 13 \quad 2 - 14 \quad 3 - 7 \quad 4 - 11 \quad 5 - 12 \quad 7 - 17 \quad 9 - 10 \quad 18 - 30 \quad 19 - 31 \quad 20 - 24 \quad 21 - 28 \quad 22 - 29 \quad 24 - 46 \quad 20 - 24 \quad 20$ 26-27 35-54 35-55 36-52 36-53 37-58 37-59 39-56 39-57 42-62 42-63 44-64 44-65 47-60 47-61 normalized bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 18-19 \quad 18-23 \quad 19-20 \quad 20-21 \quad 21-22 \quad 22-23$ Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:Atom 35:CLASS 36:Atom 37:Atom 38:Atom 40:CLASS 41:CLASS 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:CLASS 49:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:CLASS 64:CLASS 65:CLASS fragments assigned product role: containing 18 fragments assigned reactant/reagent role: containing 1 containing 34 L1 STRUCTURE UPLOADED => FS L1 FULL FS IS NOT A RECOGNIZED COMMAND The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>). => S L1 FULL FULL SEARCH INITIATED 10:43:37 FILE 'CASREACT' SCREENING COMPLETE -2 REACTIONS TO VERIFY FROM 2 DOCUMENTS 100.0% DONE 2 VERIFIED 0 HIT RXNS 0 DOCS SEARCH TIME: 00.00.01 0 SEA SSS FUL L1 (0 REACTIONS) L2=> ---Logging off of STN---=> Executing the logoff script... => LOG Y SINCE FILE COST IN U.S. DOLLARS TOTAL

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